

OPTIMAL CONTROL OF THE STATIONARY QUANTUM DRIFT-DIFFUSION MODEL IN THE SEMI-CLASSICAL LIMIT

RENÉ PINNAU, SEBASTIAN RAU, FLORIAN SCHNEIDER AND OLIVER TSE

ABSTRACT. We consider an optimal control problem of the quantum drift-diffusion equation. The existence and uniqueness of solutions to the state system is shown. The control problem is then formulated as a constrained optimization problem and the existence of a minimizer is proven. The adjoint equations are derived and allow for an easy calculation of the gradient of the reduced cost functional. The existence and uniqueness of solutions for the adjoint system is also investigated. Numerical results for different cost functionals show the feasibility of our approach.

1. INTRODUCTION

Semiconductors are part of most electrical devices and are used to build different components such as transistors, photovoltaic cells and diodes. Transistors switch or amplify electrical signals, while photovoltaic cells convert the energy of light, into electricity, and a diode lets an electrical signal pass only in one direction, which is utilized in light-emitting-diodes (LEDs), see [31, 20, 29] for an overview.

Since electrical properties of a semiconductor are in between those of an isolator and a conductor, they can be manipulated by implanting impurities into the semiconductor crystal, i.e. by adding crystals that either have a lack (so-called *p-doping*) or a surplus (*n-doping*) of electrons. Therewith one can influence the conductivity and crystalline structure of the semiconductor. The task of an engineer in semiconductor industry is to build a semiconductor with the desired properties at reasonable development costs. For instance, one could desire to obtain a low leakage current in the off-state to maximize battery lifetime, and a high driving current in the on-state [28, 27]. Due to the ongoing miniaturization of semiconductor devices the need to include quantum effects arises.

One usually uses stationary models such as the stationary (classical) and quantum drift-diffusion equations [2, 4, 9, 11, 21], as well as the (classical) and quantum energy transport model [6, 14, 15] for simulating semiconductor devices. Since the quantum drift-diffusion model only differs from the drift-diffusion model by an additional term called the *Bohm potential* $\varepsilon^2 \frac{\Delta \sqrt{n}}{\sqrt{n}}$, with n being the electron density and ε^2 denotes the squared scaled Planck constant, it is natural to investigate the asymptotic behaviour for $\varepsilon \rightarrow 0$, the so-called semi-classical limit, i.e. the transition from quantum to classical regime.

A result for the semi-classical limit of the quantum drift-diffusion equations is known (cf. [1]). The result states that every sequence of solutions of the quantum drift-diffusion equations contains a subsequence which converges weakly in $H^1(\Omega)$ to a solution of the drift-diffusion equations. We will use the idea of this result to show that minima and minimizers of a quantum drift-diffusion constrained optimal control problem converge to minima and minimizers of the classical counterpart.

2010 *Mathematics Subject Classification.* ???
Key words and phrases. ???

For this cause, we will use the concept of Γ -convergence as described in [18]. Our strategy is the following: We begin by showing that the characteristic functions for the set of solutions to the quantum drift-diffusion equations Γ -converge to the characteristic function of a set of well-behaved solutions to the drift-diffusion equations. By including the characteristic functions into the cost functionals and assuming a special structure of the cost functionals, we obtain the Γ -convergence of the functionals in the semi-classical limit. Together with the equi-coercivity of the functionals, we then obtain the convergence of minima and minimizers.

In Section 1 we introduce the state system and corresponding existence and regularity results. Then the optimal control problem is formulated and the existence of minimizers is shown. The basic concept of Γ -convergence is briefly outlined in Section 3, followed by its application to our optimal control problem where we show the convergence of minimizers and minima. Finally, those analytical results are underlined by several numerical examples.

2. STATE SYSTEM

Before stating the quantum drift diffusion equations, we impose the following assumptions on the domain, its boundary and the boundary data (see also [9, 30]):

- Assumption 2.1.** (1) Let $\Omega \subset \mathbb{R}^d$, $d \in \{1, 2, 3\}$ be a Lipschitz domain. The boundary $\partial\Omega$ splits into two disjoint parts Γ_N and Γ_D . The set Γ_D is assumed to have non-vanishing $(d-1)$ -dimensional Lebesgue measure and Γ_N is closed.
- (2) Let $\Gamma_D = \bigcup_{i=1}^M \Gamma_D^i$, $M \geq 2$ and $\text{dist}(\Gamma_D^i, \Gamma_D^j) > 0$ for $i \neq j$.
- (3) Let $\rho_D, V_D, S_D \in H^1(\Omega) \cap L^\infty(\Omega)$ with $\inf \rho_D > 0$.

Remark 2.2. The assumption above requires that any two Dirichlet boundaries Γ_D^i and Γ_D^j , $i \neq j$ be separated by some insulating part. From the physical point of view this requirement is reasonable since it prevents short-circuiting.

The quantum drift diffusion equations are given by

$$\begin{aligned} (1a) \quad & -\varepsilon^2 \Delta \rho + \rho(h(\rho) + V - S) = 0, \\ (1b) \quad & -\lambda^2 \Delta V = \rho^2 - C, \\ (1c) \quad & -\text{div}(\rho^2 \nabla S) = 0. \end{aligned}$$

on Ω with the boundary data

$$\begin{aligned} (1d) \quad & \rho = \rho_D, \quad V = V_D, \quad S = S_D \quad \text{on } \Gamma_D, \\ (1e) \quad & \partial_\nu \rho = \partial_\nu V = \rho^2 \partial_\nu S = 0 \quad \text{on } \Gamma_N, \end{aligned}$$

where ν denotes the outer normal, the variable ρ denotes the square root of the *electron density* n , i.e. $\rho := \sqrt{n}$, S the *quasi-Fermi potential* and V the *electrostatic potential* induced by the electron density and the doping profile C , which is our control parameter. The enthalpy function $h(\rho)$ accounts for electron-electron interactions and is required to satisfy the following assumption.

Assumption 2.3. Let $h \in C^1(\mathbb{R}_{>0}; \mathbb{R})$ be strictly monotone increasing with the derivative h' bounded away from zero, and $h(t) \in \mathcal{O}(t^{\frac{4}{3}})$ for $t \rightarrow \infty$. Furthermore, for any $t \in \mathbb{R}_{>0}$, let the function $r_t(\eta) = h(t + \eta) - h(\eta) - h'(t)\eta$ satisfy

$$|r_t(\eta) - r_t(\xi)| \leq L\delta|\eta - \xi|,$$

for any $\eta, \xi \in \mathbb{R}$ with $|\eta|, |\xi| \leq \delta$ for some constants $L > 0$ and $\delta > 0$.

Example 2.4. An enthalpy function that satisfies Assumption 2.3 is given by

$$h(t) := \begin{cases} T_0 \log(t), & t \leq t_0, \\ g(t), & t \geq t_0, \end{cases} \quad \text{for } t_0, T_0 > 0,$$

where g satisfies the above assumption. Furthermore, the interpolating inequalities $T_0 \log(t_0) = g(t_0)$ and $T_0 = g'(t_0)t_0$ need to be satisfied.

The expression $T_0 \log(t)$ is often used as an interaction term for low densities. However, an asymptotic expansion of exchange-correlation terms based on Fermi–Dirac statistics yields (cf. [1, 16])

$$h(t) = \mathcal{O}(t^{\frac{4}{3}}) \quad \text{for } t \rightarrow \infty.$$

This expansion basically means that the interaction term grows with a certain speed which is faster than the logarithmic expression for low densities. This property is essential in Section 4 when using a Stampaccia argument to derive the uniform boundedness in $\varepsilon > 0$ for the potential V .

In the sequel we will use the following shorthand notations

$$\begin{aligned} H_0^1(\Omega \cup \Gamma_N) &:= \overline{C_c^\infty(\Omega \cup \Gamma_N)}^{\|\cdot\|_{H^1(\Omega)}}, \\ \mathcal{Y}_0 &:= H_0^1(\Omega \cup \Gamma_N) \cap L^\infty(\Omega), \quad \|\cdot\|_{\mathcal{Y}_0} := \|\cdot\|_{H^1(\Omega)} + \|\cdot\|_{L^\infty(\Omega)}, \\ \mathcal{Y}_1 &:= \rho_D + \mathcal{Y}_0, \quad \mathcal{Y}_2 := V_D + \mathcal{Y}_0, \quad \mathcal{Y}_3 := S_D + \mathcal{Y}_0, \\ \mathcal{Y} &:= \mathcal{Y}_1 \times \mathcal{Y}_2 \times \mathcal{Y}_3, \end{aligned}$$

and the admissible set

$$\mathcal{C} := \{C \in H^1(\Omega) \mid C = C_{\text{ref}} \text{ on } \partial\Omega\},$$

with a given reference doping profile $C_{\text{ref}} \in H^1(\Omega) \cap L^\infty(\Omega)$.

2.1. Preliminary results. It is convenient to write system (1) as a single equation with the help of solution operators.

To incorporate the inhomogeneous Poisson equation (1b), we define the solution operator $\Phi : L^2(\Omega) \mapsto \mathcal{Y}_0$; $f \mapsto \Phi[f]$ as the unique weak solution of

$$-\lambda^2 \Delta \Phi = f \quad \text{in } \Omega, \quad \Phi = 0 \quad \text{on } \Gamma_D, \quad \partial_\nu \Phi = 0 \quad \text{on } \Gamma_N,$$

and $\Phi_e \in \mathcal{Y}_2$ as the unique weak solution of

$$-\lambda^2 \Delta \Phi_e = 0 \quad \text{in } \Omega, \quad \Phi_e = V_D \quad \text{on } \Gamma_D, \quad \partial_\nu \Phi_e = 0 \quad \text{on } \Gamma_N.$$

Then we can write $V = \Phi_V[\rho^2 - C] := \Phi[\rho^2 - C] + \Phi_e$ with $\Phi_V : L^2(\Omega) \rightarrow \mathcal{Y}_2$.

Similarly, the Fermi potential S can be written as $S = \Phi_S[\rho^2]$ where the solution operator $\Phi_S : L^\infty(\Omega) \rightarrow \mathcal{Y}_3$ is defined as the unique weak solution of

$$-\text{div}(\rho^2 \nabla \Phi_S) = 0 \quad \text{in } \Omega, \quad \Phi_S = S_D \quad \text{on } \Gamma_D, \quad \rho^2 \partial_\nu \Phi_S = 0 \quad \text{on } \Gamma_N,$$

for $\rho \geq \underline{\rho}$ almost everywhere in Ω for some constant $\underline{\rho} > 0$.

The solution operators Φ, Φ_e and Φ_S are well defined due to standard elliptic theory [7]. Consequently, we may write the weak solutions of system (1) as solutions of the operator equation

$$(2) \quad e_\varepsilon(\rho, C) = 0 \quad \text{in } H^1(\Omega)^*,$$

where the nonlinear operator $e_\varepsilon : \mathcal{Y}_1 \times \mathcal{C} \rightarrow H^1(\Omega)^*$ is given by

$$\langle e_\varepsilon(\rho, C), \varphi \rangle := \langle -\varepsilon^2 \Delta \rho + \rho(h(\rho) + \Phi_V[\rho^2 - C] - \Phi_S[\rho^2]), \varphi \rangle \quad \forall \varphi \in H^1(\Omega).$$

We recall existence results and a priori estimates to (1) shown in [1, 11, 30]:

Proposition 2.5. *Let Assumption 2.1 be satisfied. Then for any $C \in \mathcal{C}$ and every data (ρ_D, V_D, S_D) with*

$$1/K \leq \rho_D \leq K \quad \text{a.e. in } \Omega, \quad \|V_D\|_{L^\infty(\Omega)}, \|S_D\|_{L^\infty(\Omega)} \leq K$$

for some $K \geq 1$, there exists $(\rho, V, S) \in \mathcal{Y}$ with $V := \Phi_V[\rho^2 - C]$ and $S := \Phi_S[\rho^2]$ satisfying (2) and the estimates

$$(3) \quad \rho \geq 1/L \quad \text{a.e. in } \Omega, \quad \|\rho\|_{\mathcal{Y}_1} + \|V\|_{\mathcal{Y}_2} + \|S\|_{\mathcal{Y}_3} \leq L,$$

for some constant $L = L(\Omega, K, \|C\|_{L^p(\Omega)}) \geq 1$, where $H^1(\Omega) \hookrightarrow L^p(\Omega)$ holds.

Remark 2.6. Solutions of system (1) can be related to the extrema of the quantum energy defined by the functional

$$(4) \quad E_S^\varepsilon(\rho) := \varepsilon^2 \int_\Omega |\nabla \rho|^2 dx + \int_\Omega H(\rho) dx + \frac{\lambda^2}{2} \int_\Omega |\nabla V|^2 dx - \int_\Omega S \rho^2 dx$$

where $H(t) := \int_1^t h(s) ds$ and $C \in \mathcal{C}$, $S \in \mathcal{Y}_3$ are given. If $(\rho, V, S) \in \mathcal{Y}$ is the solution from Proposition 2.5, then ρ is a minimizer of E_S^ε in \mathcal{Y}_1 . Furthermore, ρ is the unique minimizer (for fixed S) since E_S^ε is strictly convex, see [1, 30].

One drawback is that the solution from Proposition 2.5 need not be unique. Uniqueness may be assured for small applied voltages U (see Proposition 6.1 below) and is essential when formulating an optimization algorithm. However, uniqueness is not required for the purpose of this paper.

3. OPTIMIZATION PROBLEM

We state the optimization problem with a general cost functional \mathcal{J} satisfying the following assumptions.

Assumption 3.1. Let $J: H^1(\Omega) \times \mathcal{C} \rightarrow \mathbb{R}$ denote a cost functional which is continuously Fréchet differentiable with Lipschitz continuous derivatives, bounded from below, and radially unbounded with respect to the second variable. Furthermore, let J be of separated type, i.e. we can write $J(\rho, C) = J_a(\rho) + J_b(C)$ with $J_a: H^1(\Omega) \rightarrow \mathbb{R}$ being weakly continuous and J_b being weakly lower semicontinuous in $H^1(\Omega)$.

Example 3.2. For example, the cost functional

$$(5) \quad J_1(\rho, C) := \frac{1}{2} \|\rho^2 - n_d\|_{L^2(\Omega)}^2 + \frac{\gamma}{2} \|\nabla(C - C_{\text{ref}})\|_{L^2(\Omega)}^2$$

satisfies Assumption 3.1 due to the compact Sobolev embedding $H^1(\Omega) \hookrightarrow L^p(\Omega)$, $p \in [1, 6)$ up to $d = 3$. Therefore the tracking type term is continuous with respect to the weak topology in $H^1(\Omega)$, and the second term is weakly lower semicontinuous since the norm is weakly lower semicontinuous.

Example 3.3. Another cost functional often used for the optimal design of a semiconductor by tracking the total current on the boundary is

$$(6) \quad J_2(\rho, C) := \frac{1}{2} |I(\rho) - I_d|^2 + \frac{\gamma}{2} \|\nabla(C - C_{\text{ref}})\|_{L^2(\Omega)}^2$$

where the total current $I(\rho)$ is given by

$$I(\rho) := \int_{\Gamma_O} \rho^2 \partial_\nu \Phi_S[\rho^2] ds,$$

where ν is the outer normal and $\Gamma_O \subset \Gamma_D$. Unfortunately, this functional does not satisfy Assumption 3.1 due to the boundary integral and the lack of an appropriate embedding for the trace operator.

Now we can formulate the optimization problem:

Problem 1. Let J satisfy Assumption 3.1. The optimal control problem reads: Find $(\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$ such that

$$J(\rho_*, C_*) = \min_{(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C}} J(\rho, C) \quad \text{s.t.} \quad e_\varepsilon(\rho, C) = 0 \quad \text{in } H^1(\Omega)^*.$$

The existence of a minimizer for any cost functional satisfying Assumption 3.1 is a consequence of the existence results and apriori bounds of Proposition 2.5.

Theorem 3.4. *There exists at least one solution $(\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$ to Problem 1.*

Proof. Since J is bounded from below we can define

$$j := \inf_{(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C}} J(\rho, C) > -\infty.$$

Now we choose a minimizing sequence (ρ_k, C_k) . From the radial unboundedness of J with respect to C we get a uniform bound for $(C_k) \subset H^1(\Omega)$. Since (C_k) is also uniformly bounded in $L^\infty(\Omega)$, the apriori estimate (3) yields the uniform boundedness of $(\rho_k) \subset \mathcal{Y}_1$. We can therefore deduce the existence of a subsequence, again denoted by (ρ_k, C_k) , and a $(\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$ such that

$$\rho_k \rightharpoonup \rho_* \quad \text{in } H^1(\Omega), \quad \rho_k \rightharpoonup^* \rho_* \quad \text{in } L^\infty(\Omega), \quad C_k \rightharpoonup C_* \quad \text{in } H^1(\Omega).$$

These convergences are sufficient to pass to the limit in the weak formulation. We begin with the term ρ^2 . From the weak convergence in $H^1(\Omega)$ we deduce for $p < 6$ the strong convergence of a subsequence of (ρ_k) in $L^p(\Omega)$, and consequently yet another subsequence (denoted again by (ρ_k)) that converges a.e. in Ω , i.e.,

$$\rho_k(x) \rightarrow \rho_*(x) \quad \text{a.e. in } \Omega.$$

Therefore, passage to the limit in the nonlinear terms ρ^2 and $\rho h(\rho)$ may be shown by a simple application of the Lebesgue dominated convergence. Also in the other terms, the above convergences are sufficient to pass to the limit. Indeed, by defining $V_k := \Phi_V[\rho_k^2 - C_k]$, and $S_k := \Phi_S[\rho_k^2]$, we obtain from estimate (3)

$$S_k \rightharpoonup S_* \quad \text{in } H^1(\Omega), \quad V_k \rightharpoonup V_* \quad \text{in } H^1(\Omega)$$

for some $V_* \in \mathcal{Y}_2$ and $S_* \in \mathcal{Y}_3$. The continuity and linearity of Φ_V allows to identify $V_* = \Phi_V[\rho_*^2 - C_*]$. As for S_* , we use the Lebesgue dominated convergence again to show the strong convergence of $\rho_k^2 \nabla \varphi \rightarrow \rho_*^2 \nabla \varphi$ in $L^2(\Omega)$ for any $\varphi \in H^1(\Omega)$, and consequently the convergence

$$(\rho_k^2 \nabla S_k, \nabla \varphi) = (\nabla S_k, \rho_k^2 \nabla \varphi) \rightarrow (\nabla S_*, \rho_*^2 \nabla \varphi) \quad \text{for } k \rightarrow \infty, \quad \forall \varphi \in H^1(\Omega),$$

which implies that $S_* = \Phi_S[\rho_*^2]$. Altogether, we obtain

$$0 = \langle e_\varepsilon(\rho_k, C_k), \varphi \rangle \rightarrow \langle e_\varepsilon(\rho_*, C_*), \varphi \rangle \quad \forall \varphi \in H^1(\Omega).$$

By standard arguments due to the weak lower semicontinuity of J , we finally conclude that $(\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$ solves the minimization problem (1). \square

4. Γ -CONVERGENCE FOR THE SEMI-CLASSICAL LIMIT

As mentioned earlier, we will use the concept of Γ -convergence to prove the convergence of minima and minimizers in the semi-classical limit. An introduction into this topic may be found, for example, in [3, 18]. In essence, Γ -convergence of functionals can be characterized by the following two inequalities, the so called liminf-inequality and limsup-inequality, as given in the following proposition.

Proposition 4.1 (Γ -convergence of functionals). *Let X be a metric space and (F_n) be a sequence of functionals from X into $\overline{\mathbb{R}}$. Then (F_n) Γ -converges to F if the following two conditions are satisfied:*

- (i) For every $x \in X$ and for every sequence $(x_n) \in X$ converging to x it holds
 (L-inf)
$$F(x) \leq \liminf_{n \rightarrow \infty} F_n(x_n).$$
- (ii) For every $x \in X$ there exists a sequence $(x_n) \in X$ converging to x such that
 (L-sup)
$$F(x) \geq \limsup_{n \rightarrow \infty} F_n(x_n).$$

We will also need the *equi-coercivity* of functionals on metric spaces:

Definition 4.2 (Equi-coercivity). Let X be a metric space. A sequence (F_n) is said to be **equi-coercive** on X , if for every $t \in \mathbb{R}$ there exists a compact subset K_t of X such that $\{F_n \leq t\} \subseteq K_t$ for every $n \in \mathbb{N}$.

Altogether, it holds [3]:

Γ -convergence + equi-coercivity \Rightarrow convergence of minima and minimizers.

We apply this concept to our semi-classical limit problem. Set $X := H^1(\Omega) \times H^1(\Omega)$ to be endowed with its weak topology. Notice that X as a product of reflexive Banach spaces is again a reflexive Banach space. Moreover, for each $\varepsilon > 0$, we define Ξ_ε as the set of all admissible pairs,

$$\Xi_\varepsilon := \{(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C} \mid e_\varepsilon(\rho, C) = 0 \text{ in } H^1(\Omega)^*\},$$

and let $\chi_\varepsilon : X \rightarrow \overline{\mathbb{R}}$, be its characteristic function, given by

$$\chi_\varepsilon(\rho, C) = \begin{cases} 0 & \text{if } (\rho, C) \in \Xi_\varepsilon, \\ +\infty & \text{otherwise.} \end{cases}$$

To define the set of admissible pairs Ξ_0 for classical solutions, we first make the following Assumption:

Assumption 4.3. Let $(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C}$ with $e_0(\rho, C) = 0$. Then ρ is isolated.

In the following, we restrict the classical solution space to

$$\Xi_0 := \{(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C} \mid (\rho, C) \text{ satisfies Assumption 4.3}\}.$$

Remark 4.4. Note that $\Xi_0 \neq \emptyset$ due to existence results in [1]. Moreover, the classical analogue to the quantum energy (4) is given as

$$(7) \quad E_S^0(\rho) := \int_{\Omega} H(\rho^2) dx + \frac{\lambda^2}{2} \int_{\Omega} |\nabla V|^2 dx - \int_{\Omega} S \rho^2 dx,$$

for given $S \in \mathcal{Y}_3$. It is well-known, that if $(\rho, V, S) \in \mathcal{Y}$ solves the drift-diffusion equations, then ρ is the unique minimizer of E_S^0 in \mathcal{Y}_1 (cf. [1]).

Thus, the task at hand is to prove the following theorem:

Theorem 4.5. Let Ξ_ε and Ξ_0 be as defined above, and let (ε_n) be a sequence with $\varepsilon_n \rightarrow 0$ as $n \rightarrow \infty$. Then (χ_{ε_n}) Γ -converges to χ_0 .

For the proof of Theorem 4.5, we will need the following two lemmata, whose proof are found in Appendix A and B, respectively.

Lemma 4.6. Let (ε_n) be a sequence with $\varepsilon_n \rightarrow 0$ for $n \rightarrow \infty$ and (x_n) be a sequence with $x_n = (\rho_h, C_n) \in \Xi_{\varepsilon_n}$ for all $h \in \mathbb{N}$. If the sequence (C_n) is bounded in $H^1(\Omega)$, then the sequences (ρ_n) , $(V_n = \Phi_V[\rho_n^2 - C_n])$ and $(S_n = \Phi_S[\rho_n^2])$ are uniformly bounded in h , i.e. there exists a constant $M > 0$ independent of h such that

$$(8) \quad \|\rho_h\|_{\mathcal{Y}_1} + \|V_n\|_{\mathcal{Y}_2} + \|S_n\|_{\mathcal{Y}_3} \leq M \quad \forall n \in \mathbb{N}.$$

Furthermore, there exist uniform lower and upper bounds $0 < \underline{\rho} < \bar{\rho}$ with

$$(9) \quad \underline{\rho} \leq \rho_n \leq \bar{\rho} \quad \text{a.e. in } \Omega, \forall n \in \mathbb{N}.$$

As a result of Lemma 4.6, one may extract subsequences in (ε_n) that converge to some weak limit in X , and hope to classify the limit as a solution of the classical drift-diffusion equations. A similar result was shown in [1].

Lemma 4.7. *Let $(\rho_0, C) \in \Xi_0$ satisfy Assumption 4.3. Then there exists a sequence (ε_n) with $\varepsilon_n \rightarrow 0$ as $n \rightarrow \infty$ and a sequence (ρ_n) with $(\rho_n, C) \in \Xi_{\varepsilon_n}$ for all $n \in \mathbb{N}$ such that $\rho_n \rightharpoonup \rho_0$ in $H^1(\Omega)$.*

The idea of the proof of Lemma 4.7 lies in the fact that the quantum model is a regular perturbations of the classical model for sufficiently small $\varepsilon > 0$. Therefore, standard tools from asymptotic analysis and the implicit function theorem allows to construct solutions to the quantum model, with the help of solutions satisfying Assumption 4.3. For completeness, we include a simple proof in Appendix B.

Proof of Theorem 4.5. We need to show (L-inf) and (L-sup) of Proposition 4.1.

We begin with (L-inf): Let $x = (\rho, C) \in \Xi_0$, i.e. $\chi_0(x) = 0$. Since the characteristic function χ_0 only takes the values 0 and $+\infty$, the inequality is satisfied trivially. Now suppose $x \notin \Xi_0$, i.e. $\chi_0(x) = +\infty$. Let (x_n) be a sequence converging weakly to x in X . Suppose otherwise, i.e., $\liminf_{n \rightarrow \infty} \chi_{\varepsilon_n}(x_n) = 0$. Consequently, there exists a subsequence, again denoted by (x_n) , with $x_n \in \Xi_{\varepsilon_n}$ for all $n \in \mathbb{N}$. From the weak convergence we obtain the boundedness of the sequence in X , i.e.

$$\|\rho_n\|_{\mathcal{X}} + \|C_n\|_{\mathcal{X}} \leq c \quad \forall n \in \mathbb{N},$$

for some $c > 0$. Since ρ_n is uniformly bounded in $H^1(\Omega)$, we may pass to the limit in the first term on the right hand side of (2), i.e.

$$\varepsilon_n^2 (\nabla \rho_n, \nabla \varphi)_{L^2(\Omega)} \rightarrow 0 \quad \text{for } n \rightarrow \infty.$$

Furthermore, we infer from Lemma 4.6 the existence of yet another subsequence, denoted again by (x_n) , that converges weakly to $x_* = (\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$. with

$$\begin{aligned} \rho_n &\rightharpoonup \rho_* \quad \text{in } H^1(\Omega), \quad C_n \rightharpoonup C_* \quad \text{in } H^1(\Omega), \\ \rho_n(x) &\rightarrow \rho_*(x) \quad \text{a.e. in } \Omega, \quad \rho_n \rightharpoonup^* \rho_* \quad \text{in } L^\infty(\Omega). \end{aligned}$$

As for the remaining terms in (2) we can proceed as in the proof of Theorem 3.4 to conclude the convergence

$$\langle e_0(x_*), \varphi \rangle = 0 \quad \forall \varphi \in H^1(\Omega) \implies x_* \in \Xi_0.$$

which contradicts our assumption $x \notin \Xi_0$, due to the uniqueness of weak limits. Therefore, (L-inf) holds true.

We now show (L-sup): Let $x \notin \Xi_0$, i.e. $\chi_0(x) = +\infty$. Then (L-sup) is trivially satisfied for any sequence because χ_{ε_n} only takes either the value 0 or $+\infty$. Now let $x \in \Xi_0$, i.e. $\chi_0(x) = 0$. Due to Lemma 4.7 there exists a sequence (x_n) with $x_n = (\rho_n, C)$ weakly converging to x in X with $x_n \in \Xi_{\varepsilon_n}$, i.e. $\chi_0(x_n) = 0$ for all $n \in \mathbb{N}$. Hence, (L-sup) is also satisfied in this case. This concludes the proof. \square

5. CONVERGENCE OF MINIMA AND MINIMIZERS

To include the state equation into the cost functional we use the characteristic function and define the cost functional \mathcal{J}_ε as

$$(10) \quad \mathcal{J}_\varepsilon = J + \chi_\varepsilon,$$

where J is a functional satisfying Assumption 3.1. Problem 1 can now be formulated as follows:

Problem 2. Find $(\rho_*, C_*) \in \mathcal{Y}_1 \times \mathcal{C}$ such that

$$\mathcal{J}_\varepsilon(\rho_*, C_*) = \min_{(\rho, C) \in \mathcal{Y}_1 \times \mathcal{C}} \mathcal{J}_\varepsilon(\rho, C).$$

Remark 5.1. Note that \mathcal{J}_ε is no longer Fréchet differentiable. However, this is not crucial since Problem 1 and Problem 2 are equivalent.

To prove the Γ -convergence of $(\mathcal{J}_\varepsilon)$ to \mathcal{J}_0 , we use the fact that (χ_ε) Γ -converges to χ_0 , along with Assumption 3.1 on the cost functional J . This is sufficient to prove the Γ -convergence of $(\mathcal{J}_\varepsilon)$ to \mathcal{J}_0 .

Theorem 5.2. *Let $(\mathcal{J}_\varepsilon)$ and \mathcal{J}_0 be defined as above. Then*

$$\Gamma\text{-}\lim_{\varepsilon \rightarrow 0} \mathcal{J}_\varepsilon = \mathcal{J}_0,$$

i.e. \mathcal{J}_0 is the Γ -limit of \mathcal{J}_ε .

Proof. Let (ε_n) be a sequence with $\varepsilon_n \rightarrow 0$ for $n \rightarrow \infty$ and X be defined as in Theorem 4.5.

To see that the sequence $(\mathcal{J}_{\varepsilon_n})$ satisfies (L-inf), we note that J is weakly lower semicontinuous due to Assumption 3.1. Now let $x = (\rho, C) \in X$ and $(x_n) \in X$ be a sequence converging to x , then we can estimate

$$\mathcal{J}_0(x) = J(x) + \chi_0(x) \leq \liminf_{h \rightarrow \infty} J(x_n) + \liminf_{h \rightarrow \infty} \chi_{\varepsilon_n}(x_n) \leq \liminf_{h \rightarrow \infty} \mathcal{J}_{\varepsilon_n}(x_n),$$

which gives the liminf-inequality.

To show (L-sup) we exploit the special structure of J ensured by Assumption 3.1. Let $x = (\rho, C) \in X$. If $\mathcal{J}_0(x) = +\infty$, we define the constant sequence $x_n = x$ for all $n \in \mathbb{N}$. For sufficiently large $k \in \mathbb{N}$, we have $\mathcal{J}_{\varepsilon_n}(x_n) = +\infty$ for $n > k$, because otherwise (L-inf) would be violated. Therefore (L-sup) holds for this case. If $\mathcal{J}_0(x) < \infty$, i.e. $x \in \Xi_0$, we can argue as in the proof of Theorem 4.5 to show the existence of a sequence $(\rho_n, C) \in \Xi_{\varepsilon_n}$ converging weakly to x in X . Assumption 3.1 ensures the continuity of J with respect to the weak topology. Since the doping profile C is constant, this yields $J(x_n) \rightarrow J(x)$ as $n \rightarrow \infty$, and consequently also $\mathcal{J}_{\varepsilon_n}(x_n) \rightarrow \mathcal{J}_0(x)$ as $n \rightarrow \infty$. Thus, (L-sup) also holds in this case. \square

It remains to show the equi-coercivity of the functionals \mathcal{J}_ε , which is done with the help of Lemma 4.6.

Theorem 5.3. *The sequence $(\mathcal{J}_\varepsilon)$ is equi-coercive in X .*

Proof. Recalling Definition 4.2, we need to show that the subset $\{\mathcal{J}_\varepsilon \leq t\}$ is bounded w.r.t. the strong topology in X for every $t \in \mathbb{R}$, i.e. the norm

$$\|x\|_X = \|\rho\|_{H^1(\Omega)} + \|C\|_{H^1(\Omega)}$$

must be bounded for every $x = (\rho, C)$ with $\mathcal{J}^\varepsilon(x) \leq t$ for every $t \in \mathbb{R}$.

Let $t < \infty$. Then every $(\rho, C) \in \{\mathcal{J}_\varepsilon \leq t\}$ must be in the set of admissible states Ξ_ε for some $\varepsilon > 0$ due to the characteristic function χ_ε in the definition of the cost functionals in (10). Furthermore, $\|C\|_{H^1(\Omega)}$ must be uniformly bounded in ε due to the radial unboundedness of J w.r.t. C and because the term J_b is independent of ε . Due to Lemma 4.6 we also have the uniform boundedness of $\|\rho\|_{H^1(\Omega)}$, and therefore the equi-coercivity of the sequence $(\mathcal{J}_\varepsilon)$. \square

Now all the assumptions to show the convergence of minima are satisfied (cf. [18, Theorem 7.8]).

Proposition 5.4 (Convergence of minima). *Let $(\mathcal{J}_\varepsilon)$ and \mathcal{J}_0 be defined as above. Then \mathcal{J}_0 attains its minimum on X and*

$$\min_{x \in X} \mathcal{J}_0(x) = \lim_{\varepsilon \rightarrow 0} \min_{x \in X} \mathcal{J}_\varepsilon(x).$$

The convergence of minima allows us to also show the convergence of minimizers.

Corollary 5.5 (Convergence of minimizers). *Let \mathcal{J}_ε and \mathcal{J}_0 be defined as above, and let (ε_n) be a sequence with $\varepsilon_n \rightarrow 0$ as $n \rightarrow \infty$ and $x_n^* = (\rho_n^*, C_n^*)$ such that*

$$\mathcal{J}_{\varepsilon_n}(x_n^*) = \min_{x \in X} \mathcal{J}_{\varepsilon_n}(x).$$

Then there exists a subsequence, again denoted by (x_n^) , such that*

$$x_n^* \rightharpoonup x_0^* \quad \text{in } X$$

with $x_0^ \in \Xi_0$ and*

$$\mathcal{J}_0(x_0^*) = \min_{x \in X} \mathcal{J}_0(x),$$

i.e. x_0^ is a minimizer of \mathcal{J}_0 .*

Proof. Due to Proposition 5.4, there exists $k > 0$, $k \in \mathbb{N}$ and some constant $c > 0$ such that $\mathcal{J}_{\varepsilon_n}(x_n^*) < c$ for all $n \geq k$. Due to the equi-coercivity from Corollary 5.3, the sequence (x_n^*) contains a subsequence, again denoted by (x_n^*) , which converges weakly to some x_0^* in X . With the same arguments as in the proof of Theorem 4.5, we conclude that $x_0^* \in \Xi_0$. The assertion follows from [18, Corollary 7.20]. \square

6. NUMERICAL RESULTS

In this section we give a numerical example for the convergence of minima and minimizers. For the numerics part we solve the system

$$(11a) \quad -\varepsilon^2 \Delta \rho + \rho(h(\rho) + V + V_{\text{ext}} - S) = 0,$$

$$(11b) \quad -\lambda^2 \Delta V = \rho^2 - C,$$

$$(11c) \quad -\text{div}(\rho^2 \nabla S) = 0.$$

As enthalpy function we use

$$h(t) := 2 \log(t), \quad \text{for } t \leq K, K > 0,$$

and assume that our simulation stays always in the regime of 'low' densities, i.e. that $t < K$ always holds. This assumption is very common in semiconductor modelling (cf. [9, 30, 10]). Recall that the physical electron density is given by $n = \rho^2$.

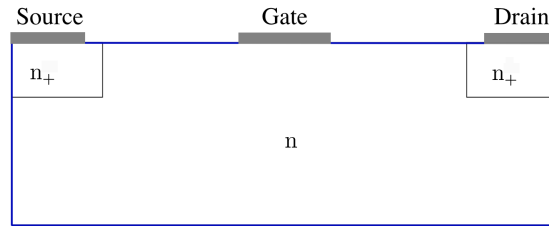


FIGURE 1. Geometry of a MESFET. The grey parts represent the Dirichlet boundary Γ_D where a potential difference is applied to source and drain. The typical gate contact controls if the MESFET is on or off. The blue lines correspond to the insulating Neumann boundary Γ_N . The n_+ region denotes the highly doped part of the MESFET while the n region is considerably less doped than the n_+ region. Taken and adapted from [13].

We intend to optimize the current of a metal semiconductor field effect transistor (MESFET) device (cf. [26]) by adjusting the background doping profile. MESFETs are typically modelled by a rectangle Ω of dimension 2 (see Fig. 1), where the boundary $\Gamma := \partial\Omega$ splits into two parts.

The Dirichlet boundary Γ_D , modelling the Ohmic contacts where an external voltage can be applied, consists of the source, drain and gate. Physically relevant boundary conditions are derived and used in [5, 17, 30]. They ensure charge neutrality and thermal equilibrium at the boundary and are given by

$$(12) \quad \rho_D = \sqrt{C}, \quad V_D = -\log\left(\frac{\rho_D^2}{\delta_c^2}\right) + U, \quad S_D = \log\left(\frac{\rho_D^2}{\delta_c^2}\right) + U,$$

where δ_c denotes the scaled intrinsic carrier concentration and U is the applied voltage at the contacts. The gate contact of the MESFET is modeled as a Schottky-contact by setting $\rho_D = \alpha_V \sqrt{C}$ for some $\alpha_V \in (0, 1)$. Here, we choose $\alpha_V = 0.1$.

For the well-posedness of the reduced cost functional

$$f(C) = J(\Phi_\rho[C], C),$$

where Φ_ρ is the control-to-state map, which assigns for any $C \in \mathcal{C}$ a unique ρ satisfying the equations (11). For this we need the uniqueness of solutions, which is ensured by the following result.

Proposition 6.1. *Let $C \in \mathcal{C}$. Then there is a constant $U_{max} > 0$ such that if*

$$\|U\|_{L^\infty(\Omega)} \leq U_{max},$$

the solution $(\rho, V, S) \in \mathcal{Y}$ from Proposition 2.5 is unique.

In the following, we will assume that the applied voltage U satisfies the assumption of Proposition 6.1. The voltage

$$(13) \quad U = \alpha_V \cdot \begin{cases} 0.15 & \text{at the drain,} \\ 0.0375 & \text{at the source,} \\ 0.075 & \text{at the gate.} \end{cases}$$

proved to be sufficiently small for the forward simulation to work.

The rest of the boundary, $\Gamma_N := \Gamma \setminus \Gamma_D$, represents the insulating parts of the boundary and is therefore of Neumann type, i.e.,

$$\partial_\nu \rho = \partial_\nu V = \rho^2 \partial_\nu S = 0,$$

where ν is the outward unit normal along Γ_N .

The aim of the optimization is to amplify the current $\rho^2 \nabla S$ over the drain $\Gamma_O \subset \Gamma_D$ to reach a given value I_d . Since it is desirable to maintain the overall structure of the semiconductor device, large deviations from the initial doping profile should be penalized. Therefore, we define the cost functional J as

$$J(\rho, S, C) = \frac{1}{2} |I(\rho, S) - I_d|^2 + \frac{\gamma}{2} \|\nabla(C - C_{\text{ref}})\|_{L^2(\Omega)}^2$$

with

$$I(\rho, S) = \int_{\Gamma_O} \rho^2 \partial_\nu S \, ds$$

where $I_d \in \mathbb{R}$ is the desired current flow on the drain Γ_O . Here, C_{ref} is the reference doping profile (e.g. the given MESFET), which is later also used as an initial guess for the optimization algorithm. The parameter $\gamma > 0$ is a regularization parameter, which allows to adjust the deviations of the optimal profile from the reference C_{ref} . This type of cost functional is most commonly used in the design of optimal doping profiles [4, 8, 9].

Remark 6.2. The Lagrange multipliers $\xi = (\xi_\rho, \xi_V, \xi_S)$ corresponding to first order optimality condition of the optimization problem are required to solve the adjoint

problem (cf. [30]), given by the equations

$$\begin{aligned} -\varepsilon^2 \Delta \xi_\rho + \xi_\rho (2 + \log(\rho^2) + V - S) \\ + 2\rho(\nabla S \cdot \nabla \xi_S - \xi_V) &= (I(\rho, S) - I_d) \nabla_S I(\rho, S) \\ -\lambda^2 \Delta \xi_V + \rho \xi_\rho &= 0 \\ -\operatorname{div}(\rho^2 \nabla \xi_S) - \rho \xi_\rho &= (I(\rho, S) - I_d) \nabla_\rho I(\rho, S) \end{aligned}$$

with homogeneous Dirichlet and Neumann boundary conditions on Γ_D and Γ_N , respectively. Since, the weak solvability of this system is a priori unknown, we will assume its solvability in $[H_0^1(\Omega \cup \Gamma_N)]^3$. In this case, the optimality condition reads

$$(15) \quad \langle f'(C_*), C - C_* \rangle \geq 0 \quad \forall C \in \mathcal{C},$$

where

$$\langle f'(C), \varphi \rangle = - \int_{\Omega} \xi_V \varphi + \gamma \nabla(C - C_d) \cdot \nabla \varphi \, dx \quad \forall \varphi \in H_0^1(\Omega).$$

For the update of the optimization algorithm, we will need the Riesz representative of the derivative denoted by $\nabla f \in H_0^1(\Omega)$. This can be done by solving the Poisson problem:

$$\text{Find } g \in H_0^1(\Omega) : \int_{\Omega} \nabla g \cdot \nabla \varphi \, dx = \langle f'(C), \varphi \rangle \quad \forall \varphi \in H_0^1(\Omega).$$

Note that $g|_{\Gamma} = 0$, therefore, if we start with some function C_0 with $C_0|_{\Gamma} = C_{\text{ref}}|_{\Gamma}$. Then the update will leave the function values on the boundary unchanged.

For the optimization we choose a gradient algorithm with line search as stated in [12]. Note that we perform an Armijo-type linesearch instead of finding the argmin along the descent direction.

Algorithm 1 Gradient Algorithm

input: A feasible doping profile $C_{\text{ref}} \in \mathcal{C}$, a tolerance $\text{TOL} > 0$.

output: A feasible doping profile C_* with (locally) minimal costs.

```

1: Set  $k = 0$ 
2: Set  $C_k = C_{\text{ref}}$ 
3: Compute gradient  $g_k = \nabla f(C_k)$ .
4: while  $\|g_k\|_{H^1(\Omega)} > \text{TOL}$  do
5:    $\alpha_k = \operatorname{argmin}_{\alpha > 0} \{f(C_k - \alpha g_k)\}$ 
6:    $C_{k+1} = C_k - \alpha_k g_k$ 
7:   Set  $k = k + 1$ 
8:   Compute gradient  $g_k = \nabla f(C_k)$ .
9: end while
10: return  $C_* = C_k$ 

```

Consider the MESFET profile:

$$C_0(x) = \begin{cases} 1 & \text{if } x \text{ is in a highly doped } n_+ \text{ region} \\ 0.01 & \text{else} \end{cases}$$

Remark 6.3. The MESFET profile C_0 is a commonly used profile in semiconductor modelling. However, it holds that $C_0 \notin \mathcal{C}$ since $C_0 \notin H^1(\Omega)$. Using this reference profile serves as a robustness check for the chosen numerical method because close to the discontinuity there occur large gradients. Nevertheless, the reference profile C_{ref} is chosen as a smoothed versions of C_0 (cf. [25])

We desire an amplification of the current of 100%, i.e. $I_d := 2I(\rho_{\text{ref}}, S_{\text{ref}})$, where ρ_{ref} and S_{ref} are computed with the reference doping profile C_{ref} . All calculations are made on a grid with 80×80 nodes and an error tolerance of 10^{-8} . We choose the parameters $\lambda^2 = 0.0017$ and $\varepsilon^2 = 1.88 \cdot 10^{-4}$. In [25] the grid independence of Algorithm 1 was also shown.

Optimization results for the quantum and classical drift-diffusion model are shown in Fig. 2. The relative deviation of the optimized doping profile to the reference profile for the quantum model can be seen in Fig. 3(a). We observe that the doping profile hardly changes in the highly doped regions and near to the contact while it is increased up to 300% in the channel. Fig. 3(c) shows that this changes the electron densities correspondingly, i.e. it varies only slightly in the upper part while it is increased up to 70% in the lower part. There is only a very small difference between the optimized profiles in the quantum and classical drift-diffusion model in Fig. 3(b). The same holds true for the electron density seen in Fig. 3(d), except close to the gate contact. In this region there occur large gradients, which are detected in the quantum model (due to the Bohm potential $\varepsilon^2 \frac{\Delta \rho}{\rho}$) but not in the classical model.

Now we investigate the semi-classical limit $\varepsilon \rightarrow 0$ numerically in more detail. Let $\varepsilon_n = \varepsilon \cdot 10^n, n = 0, \dots, 5$. Since the solutions found by Algorithm 1 might only be local minimizers and minima instead of global ones, Proposition 5.4 and Corollary 5.5 do not necessarily require them to converge. Nevertheless, from Fig. 4 we see that this is the case and that they converge to the output of Algorithm 1 for the classical model. This might be some indication that we have found global minimizers and minima.

APPENDIX A

Proof of Lemma 4.6. The idea of the proof is to derive uniform bounds for the sequences (ρ_n) , (S_n) and (V_n) in $L^\infty(\Omega)$. From this we derive a uniform bound for $\|S_n\|_{H^1(\Omega)}$, and by using the energies $E_{S_n}^{\varepsilon_n}(\rho)$ and $E_S^0(\rho)$ we derive the uniform boundedness of $\|\rho_n\|_{H^1(\Omega)}$.

So let (ε_n) and (ρ_h) be a sequences with the required properties. Using a cut-off operator, uniform bounds in n for $\|S_n\|_{L^\infty(\Omega)}$ were shown in [1], i.e. we have

$$\|S_n\|_{L^\infty(\Omega)} \leq M_1 \quad \forall h \in \mathbb{N},$$

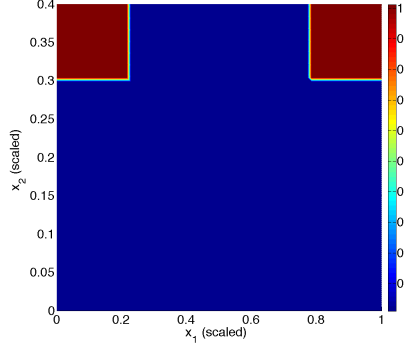
for some constant $M_1 > 0$. This yields a uniform bound for $\inf_{\rho \in \mathcal{Y}_1} E_{S_n}^{\varepsilon_n}(\rho)$. As a consequence of the asymptotic expansion $h(t) \in \mathcal{O}(t^{\frac{4}{3}})$ for $t \rightarrow \infty$ we obtain the uniform boundedness of $\|\rho_n\|_{L^{10/3}(\Omega)}$, which, together with the boundedness of the sequence (C_n) in \mathcal{C} , lead to a uniform $L^\infty(\Omega)$ bound for (V_n) (cf. [19, Section 3.2]),

$$\|V_n\|_{H^1(\Omega)} + \|V_n\|_{L^\infty(\Omega)} \leq M_2 \quad \forall n \in \mathbb{N},$$

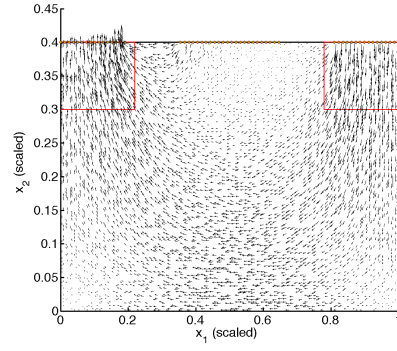
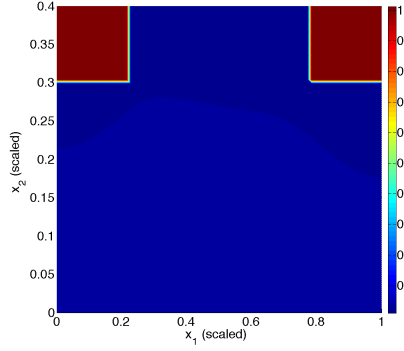
for some constant $M_2 > 0$.

To derive a uniform lower bound of ρ_n , we multiply equation (1a) with the test function $\varphi_h = \min\{0, \rho_n - \underline{\rho}\}$, where $\underline{\rho} > 0$ is a constant to be chosen appropriately. Integration by parts yields

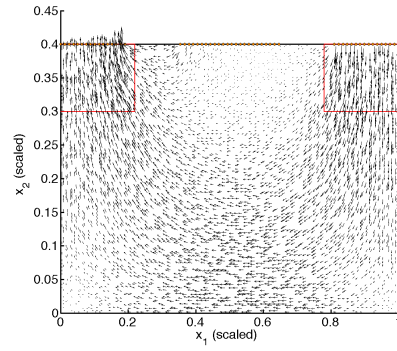
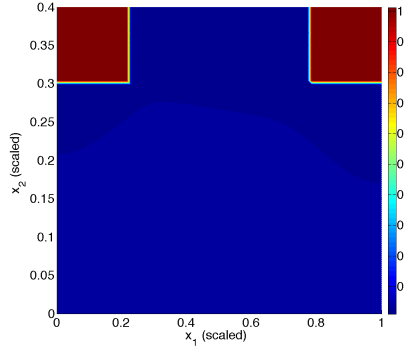
$$\begin{aligned} (16) \quad \varepsilon_h^2 \int_{\Omega} |\nabla \varphi_h|^2 dx &= - \int_{\{\rho_n \leq \underline{\rho}\}} \rho_n \varphi_h (h(\rho_n^2) + V_n - S_n) dx \\ &\leq - \int_{\{\rho_n \leq \underline{\rho}\}} \rho_n \varphi_h (h(\underline{\rho}^2) + \bar{V} - \underline{S}) dx \end{aligned}$$



(a) Reference doping profile.

(b) Total current density for reference doping profile of QDD ($\|n\nabla S\|_\infty = 0.557$).

(c) Optimized doping profile of QDD.

(d) Total current density for optimized doping profile of QDD ($\|n\nabla S\|_\infty = 0.741$).

(e) Optimized doping profile of DD.

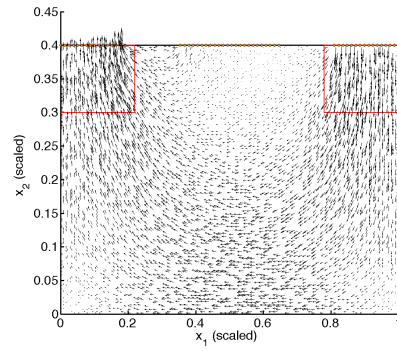
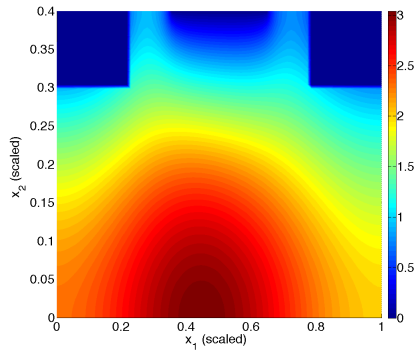
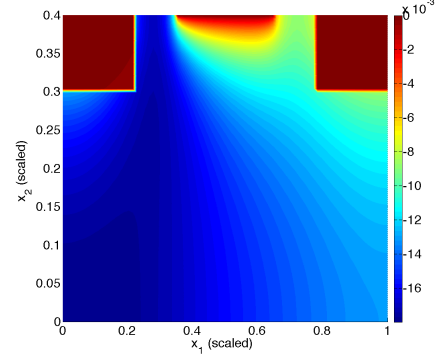
(f) Total current density for optimized doping profile of DD ($\|n\nabla S\|_\infty = 0.702$).

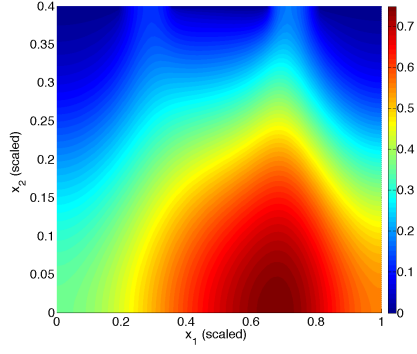
FIGURE 2. Total current densities (orange dots represent source and gate, the red rectangle the high doped n_+ region) and the reference and optimized doping profiles in the QDD and DD. For the optimization we choose the regularization parameter $\gamma = 1$.



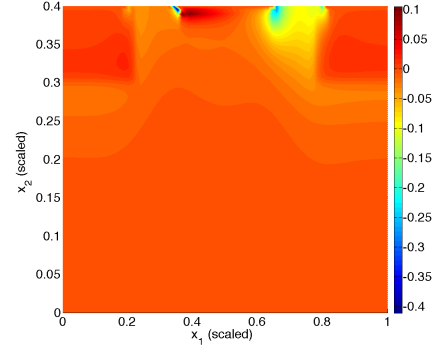
(a) Relative deviation of QDD optimized doping profile from reference doping profile.



(b) Relative deviation of QDD optimized doping profile from DD optimized doping profile.



(c) Relative deviation of the electron density for QDD optimized state from QDD reference state.



(d) Relative deviation of the electron density for QDD optimized state from DD optimized state.

FIGURE 3. Relative deviation of optimized doping profiles and electron densities to the reference solutions between QDD and DD.

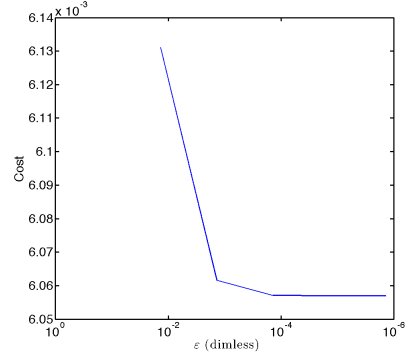
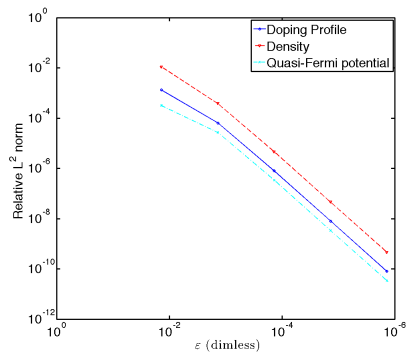


FIGURE 4. Relative L^2 -norm of doping profile, electron density and quasi Fermi potential (left) and optimal cost (right) for $\varepsilon \rightarrow 0$.

with $\bar{V} := M_2$ and $\underline{S} := \min\{0, \inf_{x \in \Omega, h \in \mathbb{N}} S_n(x)\} > -\infty$, since (S_n) is uniformly bounded in $L^\infty(\Omega)$. Now we may choose $\underline{\rho} > 0$ such that

$$h(\underline{\rho}^2) + \bar{V} - \underline{S} = 0$$

holds. Therefore, the righthand side of (16) is equal to zero. Due to the boundary conditions for (1a) we obtain

$$\varphi_h \equiv 0 \quad \text{a.e. in } \Omega, \forall n \in \mathbb{N} \implies \rho_n \geq \underline{\rho} \quad \text{a.e. in } \Omega, \forall n \in \mathbb{N}.$$

Analogously we prove the upper bound $\bar{\rho}$. Altogether we obtain

$$\underline{\rho} \leq \rho_n \leq \bar{\rho} \quad \text{a.e. in } \Omega, \forall n \in \mathbb{N}.$$

Due to $S_n = \Phi_S[\rho_n^2]$ we directly infer

$$\|S_n\|_{H^1(\Omega)} \leq M_3 \quad \forall n \in \mathbb{N},$$

for some constant $M_3 > 0$.

It remains to show the uniform $H^1(\Omega)$ bound for (ρ_n) . For some fixed $n \in \mathbb{N}$ and $S_n \in \mathcal{Y}_3$ we define the auxiliary system

$$(17a) \quad 0 = h(\tilde{\rho}_n^2) + \tilde{V}_n - S_n,$$

$$(17b) \quad -\lambda^2 \Delta \tilde{V}_n = \tilde{\rho}_n^2 - C$$

on Ω with boundary conditions

$$\tilde{\rho}_n = \rho_D, \quad \tilde{V}_n = V_D \quad \text{on } \Gamma_D, \quad \partial_\nu \tilde{\rho}_n = \partial_\nu \tilde{V}_n = 0 \quad \text{on } \Gamma_N.$$

This means that we solve the classical drift diffusion model for $(\tilde{\rho}_n, \tilde{V}_n)$ with the quantum Fermi potential S_n . Note that $(\tilde{\rho}_n, \tilde{V}_n, C)$ solves the system (17) weakly if and only if $\tilde{\rho}_n$ is the unique minimizer of $E_{S_n}^0$ in \mathcal{Y}_1 . From [1] we know that for each Fermi potential $S_n \in \mathcal{Y}_3$ there exists a minimizer $\tilde{\rho}_n$ in \mathcal{Y}_1 . Furthermore, we can find some constant $K \geq 1$ depending on $\|S_n\|_{L^\infty(\Omega)}$ such that

$$(18) \quad 1/K \leq \tilde{\rho}_n \leq K \quad \forall n \in \mathbb{N}.$$

Recall that $\|S_n\|_{L^\infty(\Omega)}$ is uniformly bounded. Due to the fact that ρ_n is a minimizer of $E_{S_n}^{\varepsilon_n}$, we may estimate

$$\begin{aligned} \varepsilon_n^2 \int_{\Omega} |\nabla \rho_n|^2 dx + E_{S_n}^0(\rho_n) &= E_{S_n}^{\varepsilon_n}(\rho_n) \leq E_{S_n}^{\varepsilon_n}(\tilde{\rho}_n) \\ &= \varepsilon_n^2 \int_{\Omega} |\nabla \tilde{\rho}_n|^2 dx + E_{S_n}^0(\tilde{\rho}_n) \leq \varepsilon_n^2 \int_{\Omega} |\nabla \tilde{\rho}_n|^2 dx + E_{S_n}^0(\rho_n), \end{aligned}$$

thereby implying that

$$\int_{\Omega} |\nabla \rho_n|^2 dx \leq \int_{\Omega} |\nabla \tilde{\rho}_n|^2 dx.$$

It remains to derive a uniform bound for $(\tilde{\rho}_n)$ in $H^1(\Omega)$.

Due to (18) and Assumption 2.3, we can define $h'_0 := \text{ess inf}_{x \in \Omega} h'(\tilde{\rho}_n^2(x))$ with $h'_0 \in (0, \infty)$. We then differentiate (17a) and multiply it with $\nabla \tilde{\rho}_n / 2\tilde{\rho}_n h'(\tilde{\rho}_n^2)$ (note that $\tilde{\rho}_n$ and h' are uniformly bounded in n away from zero). Integrating yields

$$\begin{aligned} \int_{\Omega} |\nabla \tilde{\rho}_n|^2 dx &= \int_{\Omega} \frac{1}{2\tilde{\rho}_n h'(\tilde{\rho}_n^2)} \nabla \tilde{\rho}_n \cdot \nabla (S_n - \tilde{V}_n) dx \\ &\leq \mu \int_{\Omega} \nabla \tilde{\rho}_n \cdot \nabla (S_n - \tilde{V}_n) dx \leq \mu \|\nabla \tilde{\rho}_n\|_{L^2(\Omega)} \|\nabla (S_n - \tilde{V}_n)\|_{L^2(\Omega)} \\ &\leq \mu \|\nabla \tilde{\rho}_n\|_{L^2(\Omega)} \left(\|\nabla S_n\|_{L^2(\Omega)} + \|\nabla \tilde{V}_n\|_{L^2(\Omega)} \right), \end{aligned}$$

with $\mu = K/2h'_0$ simply due to Hölder's inequality. With (18) and standard elliptic estimates [24], we obtain the uniform boundedness in n of $\|\nabla \tilde{V}_n\|_{L^2(\Omega)}$. Together

with the uniform bounds on $\|\nabla S_n\|_{L^2(\Omega)}$, this yields the existence of a constant $M_4 > 0$ such that

$$\|\tilde{\rho}_n\|_{H^1(\Omega)} \leq M_4 \quad \forall n \in \mathbb{N},$$

thereby inferring the existence of another constant $M_5 > 0$ with

$$\|\rho_n\|_{H^1(\Omega)} \leq M_5 \quad \forall n \in \mathbb{N},$$

which concludes to proof. \square

APPENDIX B

We will use a variant of the implicit function theorem to facilitate the proof.

Proposition B.1. *Let $\varepsilon_0 > 0$ and $F: Y \times [0, \varepsilon_0) \rightarrow Z$ be a mapping, where Y and Z are Banach spaces. Suppose*

- (i) *there exists $y_0 \in Y$ satisfying $F(y_0, 0) = 0$,*
- (ii) *F is Fréchet differentiable in a neighborhood of $(y_0, 0)$ such that the remainder term $R(\eta, \varepsilon) = F(y + \eta, \varepsilon) - F(y, \varepsilon) - D_y F(y, \varepsilon)[\eta]$ satisfies*

$$\|R(\eta, \varepsilon) - R(\xi, \varepsilon)\|_Z \leq L\delta\|\eta - \xi\|_Y$$

in a neighborhood of $(y_0, 0)$ for any $\eta, \xi \in Y$ with $\|\eta\|_Y, \|\xi\|_Y \leq \delta$ for some constants $L > 0$ and $\delta > 0$ independent of ε , and

- (iii) *the derivative $D_y F(y_0, 0)$ has a bounded inverse, i.e.,*

$$\|D_y F(y_0, 0)^{-1}\eta\|_Y \leq K\|\eta\|_Z \quad \text{for all } \eta \in Z.$$

Then, for sufficiently small $\varepsilon > 0$, the problem $F(y_\varepsilon, \varepsilon) = 0$ has a unique solution $y_\varepsilon \in Y$ in an ε -independent neighborhood of y_0 , and

$$\|u_\varepsilon - u_0\| = \mathcal{O}(\varepsilon) \quad \text{for } \varepsilon \rightarrow 0.$$

Proof of Lemma 4.7. Let $\rho_0 \in \mathcal{Y}_1$ be an isolated solution of the classical drift diffusion equations with a fixed doping profile $C \in \mathcal{C}$. Further, let $\varepsilon_0 > 0$, and set $Y = \mathcal{Y}$, $Z := \mathcal{X}^* \times \mathcal{X}^* \times \mathcal{X}^*$. Consider the operator equation

$$(19) \quad F(y_\varepsilon, \varepsilon) = 0 \quad \text{in } Z,$$

where $y_\varepsilon = (\rho_\varepsilon, V_\varepsilon, S_\varepsilon)$ and $F: \mathcal{Y} \times [0, \varepsilon_0) \rightarrow Z$ is defined by

$$\begin{aligned} \langle F_1(y, \varepsilon), \varphi_1 \rangle &= \varepsilon^2 \int_{\Omega} \nabla \rho \cdot \nabla \varphi_1 \, dx + \int_{\Omega} \rho (h(\rho^2) + V - S) \varphi_1 \, dx \\ \langle F_2(y, \varepsilon), \varphi_2 \rangle &= \lambda^2 \int_{\Omega} \nabla V \cdot \nabla \varphi_2 \, dx - \int_{\Omega} (\rho^2 - C) \varphi_2 \, dx \\ \langle F_3(y, \varepsilon), \varphi_3 \rangle &= \int_{\Omega} \rho^2 \nabla S \cdot \nabla \varphi_3 \, dx \end{aligned}$$

for all $\varphi = (\varphi_1, \varphi_2, \varphi_3) \in Z$. Note that the operator equation above is equivalent to the one given in (2), and the equation with $\varepsilon = 0$ corresponds to the classical drift diffusion equations. Hence, $y_0 = (\rho_0, V_0 = \Phi_V[\rho_0^2 - C], S_0 = \Phi[\rho_0^2]) \in \mathcal{Y}$ satisfies $F(y_0, 0) = 0$ in Z . We also recall the Fréchet differentiability of the operator F in a neighborhood of $(y_0, 0)$ (cf. [23]). Furthermore, due to Assumption 4.3 we deduce that the derivative $D_y F(y_0, 0)$ has a bounded inverse, i.e.,

$$\|D_y F(y_0, 0)^{-1}\eta\|_Y \leq K\|\eta\|_Z \quad \text{for all } \eta \in Z.$$

The remainder term R has the form

$$\begin{aligned} \langle R(\eta, \varepsilon), \varphi \rangle &= \int_{\Omega} [2\rho_0 \eta_\rho \nabla \eta_S + \eta_\rho^2 \nabla(S + \eta_\rho)] \cdot \nabla \varphi_1 \, dx \\ &\quad + \int_{\Omega} [\rho_0 r_\rho(\eta_\rho) + \eta_\rho (h(\rho_0 + \eta_\rho) - h(\rho_0) + \eta_V - \eta_S)] \varphi_2 \, dx - \int_{\Omega} \eta_\rho^2 \varphi_3 \, dx, \end{aligned}$$

where r_ρ is as defined in Assumption 2.3. It is an easy exercise to check that

$$\|R(\eta, \varepsilon) - R(\xi, \varepsilon)\|_{\mathcal{Z}} \leq L\delta\|\eta - \xi\|_{\mathcal{Y}}$$

for any $\eta, \xi \in \mathcal{Y}$ with $\|\eta\|_{\mathcal{Y}}, \|\xi\|_{\mathcal{Y}} \leq \delta$ for some constants $L > 0$ and $\delta > 0$. Observe that these constants are independent of ε , since R is independent of ε . We conclude the proof by applying Proposition B.1. \square

REFERENCES

- [1] N.B. Abdallah and A. Unterreiter. On the stationary quantum drift diffusion model. *Z. Angew. Math. Phys.* 49 (1998), 251-275.
- [2] M.G. Ancona and G.J. Iafrate. Quantum correction of the equation of state of an electron gas in a semiconductor. *Physical Review B*, 39(19):9536-9540, 1989.
- [3] A. Braides. *Γ -Convergence for Beginners*. Oxford University Press, New York, 2002.
- [4] M. Burger and R. Pinnau. Fast optimal design of semiconductor devices. *SIAM J. Appl. Math* 64, 108-126, 2003.
- [5] C. de Falco, E. Gatti, A. L. Lacaita, and R. Sacco. Quantum-corrected drift-diffusion models for transport in semiconductor devices. *Journal of Computational Physics*, 204(2):533 – 561, 2005.
- [6] C. Drago and R. Pinnau. Optimal dopant profiling based on energy-transport semiconductor models. *M3AS* 18(2), 195-214, 2008.
- [7] D. Gilbarg and N.S. Trudinger. *Elliptic partial differential equations of second order*. Springer, 1 edition, 1983.
- [8] M. Hinze and R. Pinnau. Mathematical tools in optimal semiconductor design. *Bulletin of the Institute of Mathematics, Academia Sinica (New Series)*, 4(2), 569-586, 2007.
- [9] M. Hinze and R. Pinnau. An optimal control approach to semiconductor design. *Math. Mod. Meth. Appl. Sc.* 12, No. 1, 89-107, 2002.
- [10] M. Hinze and R. Pinnau. A second order approach to optimal semiconductor design. *JOTA* 133, No. 2, 179-199 (2007).
- [11] M. Hinze and R. Pinnau. Optimal control of the drift diffusion model for semiconductor devices. In *Int. Ser. Num. Math.* 139, 95-106. Birkhäuser, 2001.
- [12] M. Hinze, R. Pinnau, M. Ulbrich, and S. Ulbrich. *Optimization with PDE constraints*. Springer, 2009.
- [13] S. Holst, A. Jüngel, and P. Pietra. A mixed finite-element discretization of the energy-transport model for semiconductors. *Konstanzer Schriften in Mathematik und Informatik*, 2001.
- [14] A. Jüngel, R. Pinnau, and E. Röhrig. Existence analysis for a simplified energy-transport model for semiconductors. *to appear in M3AS* (2013).
- [15] A. Jüngel, R. Pinnau, and E. Röhrig. Analysis of a bipolar energy-transport model for a metal-oxide-semiconductor diode. *JMAA* 378(2):764-774, 2011.
- [16] Ansgar Jüngel. Asymptotic analysis of a semiconductor model based on Fermi-Dirac statistics. *Math. Methods Appl. Sci.*, 19(5):401-424, 1996.
- [17] P. A. Markowich. The stationary semiconductor device equations. *Computational Microelectronics Series*, 2004.
- [18] G. Dal Maso. *An Introduction to Γ -convergence*. Birkhäuser, 1993.
- [19] C. Meyer, P. Philip, and F. Tröltzsch. Optimal control of a semilinear PDE with nonlocal radiation interface conditions. *SIAM J. Control Optim.*, 45(2):699-721 (electronic), 2006.
- [20] R. S. Muller and T. I. Kamins. *Device Electronics for Integrated Circuits*. John Wiley and Sons Australia, Limited, 3. auflage edition, 2003.
- [21] R. Pinnau. *The quantum drift diffusion model for semiconductor devices*. Shaker, Aachen, 1999.
- [22] R. Pinnau, S. Rau, and F. Schneider. Optimal quantum semiconductor design based on the quantum euler-poisson model. *Submitted* (2012).
- [23] R. Pinnau and A. Unterreiter. The stationary current-voltage characteristics of the quantum drift diffusion model. *SIAM J. Numer. Anal.* 37, No. 1, 211-245 (1999).
- [24] M. Renardy and R.C. Rogers. *An introduction to partial differential equations*. Springer, 2004.
- [25] F. Schneider. Optimal design of quantum semiconductor devices. Master's thesis, University of Kaiserslautern, 2011.
- [26] S.Selberherr. *Analysis and Simulation of Semiconductor Devices*. Springer, 1984.

- [27] M. Stockinger, R. Strasser, R. Plasun, A. Wild, and S. Selberherr. Closed-loop mosfet doping profile optimization for portable systems. *Proceedings Intl. Conf. on Modelling and Simulation of Microsystems, Semiconductors and Sensors*, 395-398, 1990.
- [28] M. Stockinger, R. Strasser, R. Plasun, A. Wild, and S. Selberherr. A qualitative study on optimized mosfet doping profiles. *Proceedings SISPAD 98 Conf.*, 77-80, 1998.
- [29] S. M. Sze. *Semiconductor devices, physics and technology*. Wiley, New York, 1985.
- [30] A. Unterreiter and S. Volkwein. Optimal control of the stationary quantum drift-diffusion model. *Communications in Mathematical Sciences*, 5:85-111, 2007.
- [31] B.G. Yacobi. *Semiconductor materials - an introduction to basic principles*. Springer, 2002. edition.